Atomistic Modeling of Shocks in Al and Cu Single Crystals

Paul H. Erhart
University of Illinois at Urbana-Champaign and Darmstadt University of Technology, Germany

Nick M. Tanushev
California Institute of Technology Pasadena, California

Eduardo M. Bringa, María-José Caturla, Brian D. Wirth
Chemistry and Materials Science, Lawrence Livermore National Laboratory, California

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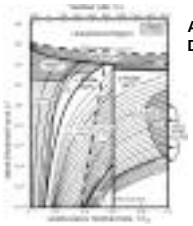
Abstract:

We present results of molecular dynamics (MD) simulations of shocks on single crystal Al and Cu samples. These results provide an important insight into the anisotropic response of single crystals and the underlying mechanisms responsible for plastic deformation. Significant experimental work has been done on the shock deformation behavior of polycrystalline samples, however, many of the underlying mechanisms responsible for material deformation at high strain-rates are not well understood. MD simulations can provide data on the formation of defects under such strains. Visualization of the data using a centro-symmetry parameter (CSP) analysis allows the identification of the defect structures formed. Our results describe the elastic Hugoniot and plastic response of single crystal Al and Cu, as well as the effect of vacancies and voids on the plastic response of the crystal. Melting is observed above shock pressures of 120 GPa in Al, in accordance with previous studies. Finally, dislocation arrays and nano-twins are identified in Cu, in good agreement with deformation microstructures observed in recent laser-driven shock experiments.



Ashby-Frost Map of Deformation Mechanisms

- Unexplored region accessible by means of MD simulations and laser-driven shock experiments
- New materials science

Methods:

- Molecular Dynamics (MD)

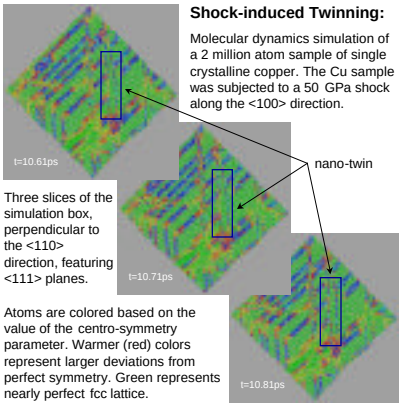
The time evolution of an initial configuration of atoms is simulated. At each time step, the force vector of every atom is computed due to its neighbors and external potential. The new positions result from integrating Classical Newtonian mechanics. Simulations were preformed using MDCask, which is a parallelized code developed at LLNL. In this code, a shock is introduced by applying a constant force to several layers of atoms at the surface of the crystal. The interatomic forces are computed using Embedded Atom Method (EAM) potentials. MDCask outputs the locations of the atom at regular intervals along with other important quantities such as the kinetic and potential energy.

- Centro-Symmetry Parameter (CSP)

Post-processing of the output is used to identify defect structures. The CSP is a good measure of the topological condition of crystals. In face-centered cubic (fcc) crystals such as Al and Cu, the CSP is defined by the magnitude of the sum of the 12 vectors defined by each atom and its nearest neighbors. For a perfect lattice, this magnitude is 0. To further aid the visualization of the crystal, we take thin slices in a given crystallographic orientation and plot them using commercial visualization packages, such as RasMol. The color of each atom is based on the magnitude of its CSP.

Shock-induced Twinning:

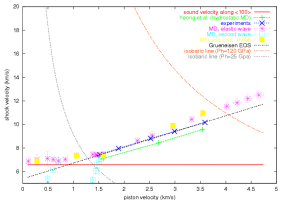
Molecular dynamics simulation of a 2 million atom sample of single crystalline copper. The Cu sample was subjected to a 50 GPa shock along the <100> direction.



Three slices of the simulation box, perpendicular to the <110> direction, featuring <111> planes.

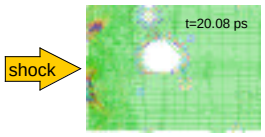
Atoms are colored based on the value of the centro-symmetry parameter. Warmer (red) colors represent larger deviations from perfect symmetry. Green represents nearly perfect fcc lattice.

Hugoniot Plot for Al <100>



Shocks along <100> between 2 and 300 GPa in perfect Al single crystals have been simulated. The forces were calculated with the Ercolessi-Adams EAM Al potential. Excellent agreement has been found with experimental Hugoniot data and the observation of melting at pressures over approx. 120 GPa is consistent with previous studies.

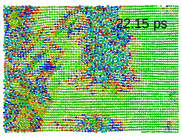
Shock at 25 GPa in Single Crystalline Al Along the <001> Direction with Approximately 5% Void Concentration:



The slides show <010> cuts of the sample, i.e. perpendicular to the direction of shock propagation. The atoms are colored according to their CSP value. Warm colors (red) correspond to large deviations from perfect crystallinity.

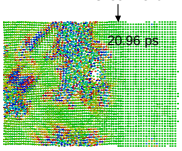
20.72 ps

The series of snapshots shows the propagation of a 25 GPa shock along the <001> direction in a Al single crystal. The initial sample contained nearly 5 % voids with an exponential size distribution.



22.72 ps

shock front



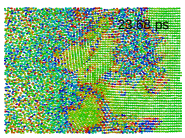
The first four slides show the closure of a void leaving behind a molten region. It can be seen that the void surfaces serve as dislocation nucleation sites. As expected in general for fcc crystals slip occurs on <111> planes.

21.5 ps

"piston"

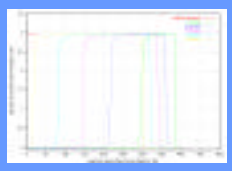
23.22 ps

dislocation



The last four slides illustrate the separation and rotation (?) of crystalline regions before the piston. The circled "nano-crystallite" is surrounded by a molten or amorphous layer and its orientation has markedly changed with respect to the original lattice.

Velocity Profile for a 75 GPa Shock in Al:



Note that after less than 2 ps, the shock profile has already reached a steady state.

Conclusion and Acknowledgements:

The MD simulations in Al and Cu single crystals have raised numerous challenging questions. In further studies, we would hope to identify the formation mechanism as well as the growth rate for nano-twins. We have found further evidence for the necessity of the development of an anisotropic equation of state. These results might motivate further experimental studies on single crystal Al and also on crystals with isolated pre-imposed defects such as voids, grain boundaries, ***etc.***

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